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Physical model of onboard hydrogen storage tank thermal behaviour during fuelling

Vladimir Molkov

Mohammad Dadashzadeh*
s.dadashzadeh@ulster.ac.uk

Dmitriy Makarov

Hydrogen Safety Engineering and Research Centre (HySAFER), Ulster University, Newtownabbey, BT37 0QB, Northern Ireland, UK

*Corresponding author.

Abstract

A physical model to simulate thermal behaviour of an onboard storage tank and parameters of hydrogen inside the tank during fuelling is described. The energy conservation equation, Abel-Noble real gas equation of state, and the entrainment theory are applied to calculate the dynamics of hydrogen temperature inside the tank and distribution of temperature through the wall to satisfy requirements of the regulation. Convective heat transfer between hydrogen, tank wall and the atmosphere are modelled using Nusselt number correlations. An original methodology, based on the entrainment theory, is developed to calculate changing velocity of the gas inside the tank during the fuelling. Conductive heat transfer through the tank wall, composed of a load-bearing carbon fibre reinforced polymer and a liner, is modelled by employing one-dimensional unsteady heat transfer equation. The model is validated against experiments on fuelling of Type III and Type IV tanks for hydrogen onboard storage. Hydrogen temperature dynamics inside a tank is simulated by the model within the experimental non-uniformity of 5 °C. The calculation procedure is time efficient and can be used for the development of automated hydrogen fuelling protocols and systems.

Keywords: Hydrogen; Fuelling; Onboard storage; Model; Validation; Fuelling protocol

Nomenclature

Symbol Parameter name Unit

A_{int}

Internal tank surface m²

b

Co-volume constant for hydrogen in Abel-Noble equation of state m³/kg

$c_{p, air}$

Specific heat capacity of air at constant pressure J/kg/K

$c_{p,g}$

Specific heat capacity of gas inside tank at constant pressure J/kg/K

$c_{p, wall}$

Specific heat capacity of tank wall (CFRP: $c_{p \text{ wall (CFRP)}}$; liner: $c_{p \text{ wall (liner)}}$) J/kg/K

D_{ext}

External tank diameter m

D_{inlet}

Nozzle diameter m

D_{int}

Internal tank diameter m

f

Friction factor

Gr_{tank}

Grashof number

g

Gravity acceleration m/s²

h_{in}

Enthalpy of gas entering tank J/kg

k_{ext}

Convective heat transfer coefficient at external surface of tank wall W/m²/K

$k_{int\ forced}$

Convective heat transfer coefficient at external surface of tank wall (forced convection) W/m²/K

$k_{int\ natural}$

Convective heat transfer coefficient at internal surface of tank wall (natural convection) W/m²/K

k_{int}

Convective heat transfer coefficient at internal surface of tank wall W/m²/K

L

Internal tank length m

\dot{m}_{ent}

Entrainment mass flow rate kg/s

\dot{m}_{inlet}

Inlet mass flow rate kg/s

\dot{m}_{inlet}^0

Initial inlet mass flow rate kg/s

M_0

Momentum flux kg m/s²

m_{ent}

Mass of gas involved in entrainment kg

m_{inlet}

Mass of gas at inlet (in the consideration of kinetic energy) kg

m_{tank}

Mass of gas in tank kg

m_{tank}^0

Initial mass of gas in tank kg

$Nu_{int\ natural}$

Nusselt number for natural convection

$Nu_{int\ forced}$

Nusselt number for forced convection

P_{tank}

Pressure of gas inside tank Pa

P_{tank}^0

Initial pressure of gas inside tank Pa

Pr

Prandtl number of gas inside tank

Q

Heat into tank from the surrounding atmosphere J

R_{H_2}

Hydrogen gas constant m² s²/K

Re_{tank}

Reynolds number inside tank

T_{amb}

Ambient temperature K

T_{tank}

Temperature of gas inside tank K

$T_{wall(ext)}$

Temperature of tank external surface K

$T_{wall(int)}$

Temperature of tank internal surface K

T_{del}

Delivery temperature of gas during fuelling K

T_{tank}^0

Initial temperature of gas inside tank K

$T_{wall(n)}$

Temperature of tank wall at the grid-point “n” K

T_{wall}^0

Initial temperature of tank wall K

t

Time s

u_{ent}

Gas velocity due to entrainment m/s

u_{inlet}

Inlet gas velocity m/s

u_{tank}

Tank gas velocity m/s

U

Total internal energy in tank J

V

Tank volume m³

Z

Hydrogen compressibility facto

β

Thermal expansion coefficient of gas 1/K

ν

Specific heats ratio

λ_{air}

Thermal conductivity of air W/m/K

λ_g

Thermal conductivity of gas W/m/K

λ_{wall}

Thermal conductivity of tank wall (CFRP: $\lambda_{wall \text{ (CFRP)}}$; liner: $\lambda_{wall \text{ (liner)}}$) W/m/K

μ_g

Dynamic viscosity of gas Pa s

ρ_{air}

Density of air kg/m³

ρ_{inlet}

Gas density at inlet kg/m³

ρ_{tank}

Gas density inside tank kg/m³

ρ_{tank}^0

Initial gas density inside tank kg/m³

ρ_{wall}

Tank wall density (CFRP: $\rho_{wall \text{ (CFRP)}}$; liner: $\rho_{wall \text{ (liner)}}$) kg/m³

Introduction

The inherently safer fuelling of onboard hydrogen composite storage container is a challenging problem. Independent on tank design and materials used for load bearing wall and liner used to limit permeation to regulated level, tank's volume, its initial and nominal working pressure (NWP), temperature of hydrogen supplied to tank, the regulation and standards [1-4] require that the temperature inside the tank doesn't exceed 85 °C, the pressure does not exceed 1.25 × NWP, i.e. 87.5 MPa for 70 MPa onboard storage tanks and the State of Charge (SOC) does not exceed 100%. The consumer expectations include the fuelling time of onboard storage of passenger car within 3 min. Longer fuelling time is acceptable for busses. The problem of fuelling control is complicated by changing pressure and temperature inside the tank and at inlet, changing diameter of fuelling nozzle to keep a required pressure ramp profile, requirements to the fuelling time, conjugate heat transfer from/to hydrogen through a tank wall to/from the ambience, use of wall and liner materials of different thermal conductivity, thermal capacity, etc.

Experimental investigation of the fuelling for arbitrary conditions is expensive and not feasible. Up to now experimental studies didn't yet end by clear and transparent fuelling protocol. Computational fluid dynamics (CFD) is a

contemporary research method to get insights into underlying physical phenomena. It helps as well to avoid carrying out numerous hazardous experiments. However, CFD simulations are not always time efficient [5] and hardly could be used as a part of automated fuelling system with a short response time. This study aims at developing and validating against published experiments a physical model for direct, i.e. no pipe from storage to dispenser and no hose from dispenser to vehicle, fuelling of onboard hydrogen storage. The validated model can be then applied for the development of scientifically substantiated hydrogen fuelling protocol for hydrogen vehicles. The model is developed in the assumption of uniform temperature inside a tank, which is a validated assumption for tank volumes and fuelling conditions in the used for the model validation experiments: 29 L volume Type IV tank [6], 40 L volume Type III tank [6], 74 L volume Type III tank [7] with the ratio of tank length to its diameter (L:D ratio) of 3.4, 3 and 2.7 respectively. The model should be applied with care for larger volume tanks compared to characteristic onboard storage tanks of tens of litres, and other fuelling conditions, e.g. slower fuelling with poor mixing of gas inside the tank. Indeed, a strong temperature non-uniformity inside a larger tank is observed during fuelling [8] and more research should be done to derive fuelling conditions providing temperature uniformity to exclude hot spots.

There are experimental, numerical and analytical studies that have been carried out on hydrogen fuelling for high-pressure gaseous hydrogen onboard storage systems. In work [9], the pressure and temperature change during the fast fuelling of a hydrogen tank (35 MPa) were measured, and the problem of heat transfer between the tank wall and hydrogen was addressed. A model was proposed in which the energy and mass conservation laws and real gas equation of state (EOS) were employed to calculate the pressure and temperature change inside the tank. The authors didn't indicate which real gas EOS was applied in their model. Based on the experimental condition of the tested tank, an approach to calculate the heat transfer coefficient between the gas and tank wall was introduced. However, it was concluded in Ref. [10] that the heat transfer coefficient depends on the thermal physical properties of the tank and the gas, and the state of the flow which are not measurable during the fuelling process in practice [9]. In our paper we will demonstrate how to model “non-measurable” parameters.

To consider heat transfer between tank wall and gas inside the tank, an unsteady heat conduction equation was introduced in study [10] to expand the thermodynamic model [9]. Assuming a constant value of heat transfer coefficients, this model was later exploited and compared against experiments with different fuelling conditions of hydrogen tank [11-13]. The use of a constant heat transfer coefficient, which value would depend on fuelling conditions and tank volume, restricts, among other factors, the predictive capability of this model. Indeed, the comparison against experiment [11] demonstrated that there is a poor agreement between the calculated gas temperature and those measured during the experiment, e.g. 8 °C–12 °C overprediction by the proposed model. This is comparatively large overprediction keeping in mind the regulated maximum temperature 85 °C inside the tank [1-4]. The deficiency of using constant heat transfer coefficient was observed in study [14], where a poor agreement between the simulated and measured temperature of gas inside a 23 L volume Type III tank, e.g. over 40 °C and 10 °C overprediction in the beginning and the middle of fuelling was observed respectively.

The heat transfer through the wall plays an important role in the predictive capability of models for fuelling and blowdown of a tank [15,16]. It changes with a tank dimensions, its material thermal properties and fuelling conditions. The convective heat transfer on a tank walls depends on the heat transfer coefficient. The availability of universal modelling approach to estimate this coefficient for arbitrary conditions is vital for hydrogen safety engineering [17]. The value of heat transfer coefficient is important for predictive simulations of such processes as fuelling and blowdown of hydrogen from a tank. Neglecting the accuracy in calculation of this parameter could adversely affect the safety design of the tank, which could result in catastrophic accidents with severe consequences [18].

In studies [5,8] the authors employed an energy balance equation in a tank and the tank wall, as well as a real gas EOS to develop a model for the prediction of temperature increase in the tank during hydrogen filling. The correlation of [17] for heat transfer coefficients between gas and tank wall was used in their model. Previously it was concluded in Ref. [17] that the model for prediction of the heat transfer coefficient is very sensitive to the tank conditions, i.e. its thermal properties, dimensions, fuelling condition, etc. The use of inlet velocity, instead of gas characteristic velocity inside the tank, to calculate the Reynolds number and corresponding Nusselt number, to obtain the heat transfer coefficient, is questionable from our point of view even it has been extensively applied up to now in modelling of fuelling process. The agreement between the model and the experiment was quite good within 4 °C in Ref. [5] because the heat transfer coefficient correlation was derived based on the fuelling experimental results of the tested tank. The authors of [5] fairly concluded that the correlation is only valid for the tested tank with its special orientation and the fuelling condition. It was also concluded that although the model accuracy can be acceptable for the low speed industrial refuelling (e.g. forklifts), faster fillings of around 3 min, which is the target for hydrogen fuelling stations, can produce higher temperature gradients, hence higher inaccuracy of the model predictions.

The thermodynamic behaviour of the compressed hydrogen tank during the fuelling has also been studied experimentally and numerically in Refs. [6,8,19-26]. The main conclusions of these studies include but not limited to:

- Further investigation on the heat transfer from hydrogen to the tank wall is required;
- Importance of publicly available database for the fuelling experiments performed for the different fuelling conditions;
- The significance of employing the real gas EOS instead of the ideal gas EOS in evaluating the thermal behaviour of a tank during the fuelling;
- The effect of lower pre-cooling temperature which results into higher average mass flow rate, state of the charge (SOC) and total mass of the gas;
- The importance of temperature homogeneities inside the tank during the filling and effect of injector configurations on this later phenomenon;

- The need for the accurate measurement of the liner temperature during the fuelling experiments by placing thermocouples in direct contact with the tank's internal surface.

The aim of this study is to develop and validate a physical model to better understand and reproduce the underlying phenomena of onboard hydrogen tank fuelling. The model can be used as a basis for creation of a predictive tool for the thermal behaviour of the system dispenser-hydrogen-tank-atmosphere during fuelling. The ultimate goal is the establishment of inherently safer and automated hydrogen fuelling protocol.

Physical model

The schematic diagram of the hydrogen storage tank during the fuelling and phenomena on its boundaries are presented in Fig. 1.

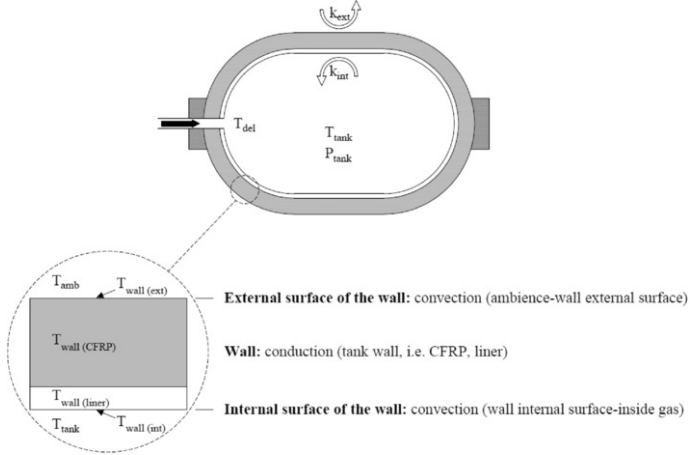


Fig. 1 Scheme of a tank and related phenomena during fuelling.

alt-text: Fig. 1

Hydrogen thermodynamic parameters during fuelling are calculated using Abel-Noble real gas EOS [27].

$$P_{tank} = Z \rho_{tank} R_{H_2} T_{tank}, \quad (1)$$

where $Z = 1/(1 - b\rho_{tank})$ is the compressibility factor.

The first law of thermodynamic is used in the model to bring together the rate of change of internal energy of hydrogen in the tank, rate of heat transfer to/from hydrogen through the tank wall, composed of the composite polymer and the liner with different thermodynamic parameters, and the rate of enthalpy brought into the tank by hydrogen inflow

$$\frac{dU}{dt} = \frac{dQ}{dt} + h_{in} \frac{dm_{tank}}{dt}, \quad (2)$$

where $h_{in} = c_{p,g} T_{del}$ is the enthalpy of the gas entering (delivered into) the tank.

The internal energy of real gas is calculated as [28].

$$U = \frac{P_{tank} (V - m_{tank} b)}{\gamma - 1}, \quad (3)$$

The rate of heat transfer can be modelled as elsewhere, e.g. Ref. [12],

$$\frac{dQ}{dt} = k_{int} A_{int} (T_{wall(int)} - T_{tank}), \quad (4)$$

where T_{tank} is the gas temperature inside the tank in the assumption of its uniformity, which is valid for onboard storage of comparatively small volume and not large length to diameter ratio (see validation experiments further

in the paper). The issue of gas temperature uniformity inside the tank should be dealt with carefully for larger volume hydrogen storage vessels and onboard tanks with large length to diameter ratios.

Convective heat transfer coefficient, k_{int} , must be calculated accurately. There could be natural, forced, or combined regime of convective heat transfer between hydrogen and internal surface of the tank wall. The criteria to define the regime of convective heat transfer are defined as [29].

$$\left\{ \begin{array}{l} \text{If } \frac{Gr_{tank}}{(Re_{tank})^2} < 0.1, \quad k_{int} = k_{int \text{ forced}}, \\ \text{If } 0.1 \leq \frac{Gr_{tank}}{(Re_{tank})^2} \leq 10, \quad k_{int} = \left(k_{int \text{ natural}}^4 + k_{int \text{ forced}}^4 \right)^{\frac{1}{4}}, \\ \text{If } \frac{Gr_{tank}}{(Re_{tank})^2} > 10, \quad k_{int} = k_{int \text{ natural}}, \end{array} \right. \quad (5-7)$$

where Grashof number, Gr_{tank} , is calculated as

$$Gr_{tank} = \frac{g\beta |T_{tank} - T_{wall(int)}| \rho_{tank}^2 D_{int}^3}{\mu_g^2}. \quad (8)$$

Table 1 presents gas thermal properties, i.e. thermal conductivity (λ_g); specific heat capacity ($c_{p,g}$); viscosity (μ_g), extracted for different pressures and temperatures from Ref. [30]. The pressure and temperature range of 0.1–77 MPa and 270–350 K, respectively, were assigned with respect to those identified in the experiments [6,7] which are used for the model validation in our study.

Table 1 Properties of hydrogen as a function of pressure and temperature [30].

alt-text: Table 1

@ T (K)	λ_g (W/m/K) @		$c_{p,g}$ (J/kg/K) @		μ_g (Pa s) @	
	P = 0.1 MPa	P = 77 MPa	P = 0.1 MPa	P = 77 MPa	P = 0.1 MPa	P = 77 MPa
270	1.71 . 10 ⁻¹	2.64 . 10 ⁻¹	1.42 . 10 ⁴	1.50 . 10 ⁴	8.33 . 10 ⁻⁶	1.12 . 10 ⁻⁵
280	1.76 . 10 ⁻¹	2.67 . 10 ⁻¹	1.42 . 10 ⁴	1.50 . 10 ⁴	8.54 . 10 ⁻⁶	1.12 . 10 ⁻⁵
290	1.81 . 10 ⁻¹	2.70 . 10 ⁻¹	1.43 . 10 ⁴	1.50 . 10 ⁴	8.75 . 10 ⁻⁶	1.13 . 10 ⁻⁵
300	1.86 . 10 ⁻¹	2.73 . 10 ⁻¹	1.43 . 10 ⁴	1.50 . 10 ⁴	8.95 . 10 ⁻⁶	1.14 . 10 ⁻⁵
310	1.91 . 10 ⁻¹	2.76 . 10 ⁻¹	1.43 . 10 ⁴	1.50 . 10 ⁴	9.16 . 10 ⁻⁶	1.15 . 10 ⁻⁵
320	1.95 . 10 ⁻¹	2.79 . 10 ⁻¹	1.44 . 10 ⁴	1.50 . 10 ⁴	9.36 . 10 ⁻⁶	1.17 . 10 ⁻⁵
330	2.00 . 10 ⁻¹	2.83 . 10 ⁻¹	1.44 . 10 ⁴	1.50 . 10 ⁴	9.56 . 10 ⁻⁶	1.18 . 10 ⁻⁵
340	2.05 . 10 ⁻¹	2.87 . 10 ⁻¹	1.44 . 10 ⁴	1.50 . 10 ⁴	9.75 . 10 ⁻⁶	1.19 . 10 ⁻⁵
350	2.10 . 10 ⁻¹	2.91 . 10 ⁻¹	1.44 . 10 ⁴	1.50 . 10 ⁴	9.95 . 10 ⁻⁶	1.20 . 10 ⁻⁵

Fig. 2 shows the developed interpolation for the hydrogen thermal properties as a function of temperature at pressures in the range from 0.1 MPa to 77.0 MPa using **Table 1** data. The interpolation calculates hydrogen properties for transient gas temperature, T_g , and pressure, P_g , in the tank.

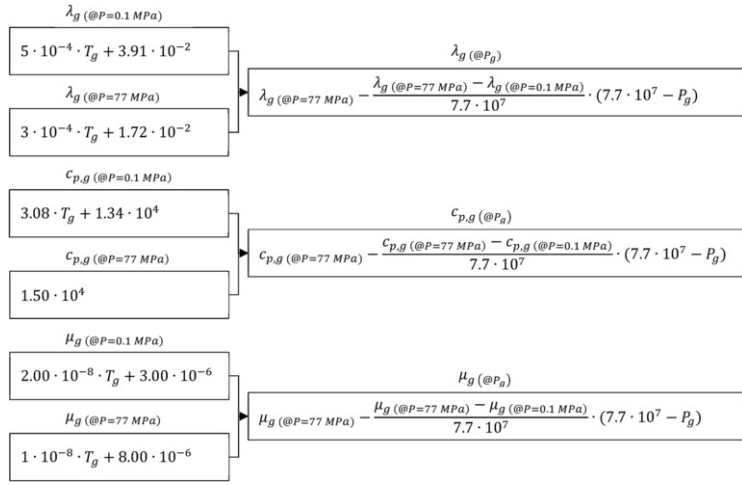


Fig. 2 The interpolation for calculation of hydrogen thermal properties as a function of temperature and pressure.

alt-text: Fig. 2

The values of heat transfer coefficients $k_{int \text{ forced}}$ and $k_{int \text{ natural}}$ are calculated as a function of Nusselt number, internal tank diameter, and gas thermal conductivity, respectively as

$$k_{int \text{ natural}} = \frac{\lambda_g \times Nu_{int \text{ natural}}}{D_{int}}, \quad (9)$$

$$k_{int \text{ forced}} = \frac{\lambda_g \times Nu_{int \text{ forced}}}{D_{int}}. \quad (10)$$

Natural convection Nusselt number, $Nu_{int \text{ natural}}$, is calculated by the empirical equation [11].

$$Nu_{int \text{ natural}} = 0.104 \times \left(\frac{g\beta |T_{tank} - T_{wall(int)}| c_{p,g} (\rho_{tank})^2 D_{int}^3}{\mu_g \lambda_g} \right)^{0.352}, \quad (11)$$

Forced convection Nusselt number, $Nu_{int \text{ forced}}$, is calculated using the correlation [29].

$$Nu_{int \text{ forced}} = \frac{(f/8) (Re_{tank} - 1000) Pr}{1 + 12.7(f/8)^{0.5} (Pr^{2/3} - 1)}, \quad (12)$$

where the friction factor, f , and Prandtl number, Pr , inside the tank are calculated by the following correlation [29] and the definition respectively

$$f = (0.790 \bullet \ln Re_{tank} - 1.64)^{-2}, \quad (13)$$

$$Pr = \frac{\mu_g \bullet c_{p,g}}{\lambda_g}. \quad (14)$$

Reynolds number inside the tank for calculation of the friction factor and Nusselt number for forced convection is

$$Re_{tank} = \frac{\rho_{tank} u_{tank} D_{int}}{\mu_g}. \quad (15)$$

The challenge in calculation of Re_{tank} is transient characteristic velocity of hydrogen inside the tank during the fuelling, u_{tank} . The original modelling approach is applied in this study to calculate the characteristic velocity of hydrogen in a tank. It is based on the entrainment theory [31], and has been previously suggested to assess the extent of uniformity of mixture inside the enclosure during hydrogen release [32]. The procedure is as follows. The density of hydrogen at inlet is calculated using Abel-Noble EOS for real gas. It was concluded in Refs. [6,33] that pressure inside the tank, P_{tank} , and pressure at inlet, P_{inlet} , are very close. Hence, P_{tank} is used to calculate the density of

hydrogen at the inlet as

$$\rho_{inlet} = \frac{P_{tank}}{P_{tank}b + R_{H_2}T_{del}}. \quad (16)$$

The inlet velocity is calculated through the equation for mass flow rate, which is in fact a parameter dependent on pressure ramp as the main input parameter of the fuelling protocol

$$u_{inlet} = \frac{4\dot{m}_{inlet}}{\rho_{inlet}(D_{inlet})^2\pi}, \quad (17)$$

Using the inlet density, ρ_{inlet} , and inlet velocity, u_{inlet} , the momentum flux, M_0 , and the entrainment mass flow rate, \dot{m}_{ent} , are calculated respectively as [31].

$$M_0 = \frac{1}{4}\pi(D_{inlet})^2\rho_{inlet}(u_{inlet})^2, \quad (18)$$

$$\dot{m}_{ent} = 0.282(M_0)^{0.5}(\rho_{tank})^{0.5}L. \quad (19)$$

Then, the velocity of hydrogen in the tank due to the entrainment process can be calculated as

$$u_{ent} = \frac{4\dot{m}_{ent}}{\rho_{tank}(D_{int})^2\pi}. \quad (20)$$

To calculate the transient characteristic velocity inside the tank, u_{tank} , the kinetic energy of hydrogen entering the tank and the kinetic energy of hydrogen moving inside the tank due to the entrainment, are added

$$\frac{m_{tank}(u_{tank})^2}{2} = \frac{m_{ent}(u_{ent})^2}{2} + \frac{m_{inlet}(u_{inlet})^2}{2}. \quad (21)$$

Considering that all hydrogen inside the tank is involved in the movement due to the entrainment phenomenon (this assumption is valid for onboard storage tanks of moderate size but should be taken carefully for storage tanks of a larger volume), i.e. $m_{ent} = m_{tank}$, and using the definition $m_{inlet} = \dot{m}_{inlet}\Delta t$, this equation can be solved for the characteristic velocity for use in the calculation of Reynolds number as

$$u_{tank} = \left[\frac{m_{tank}(u_{ent})^2 + m_{inlet}(u_{inlet})^2}{m_{tank}} \right]^{\frac{1}{2}}, \quad (22)$$

Differentiating Eq. (3) and then solving it together with Eqs. (2) and (4) the differential equation for hydrogen mass in the tank can be written as

$$\frac{dm_{tank}}{dt} = \frac{\frac{dP_{tank}}{dt} \bullet \frac{(V - m_{tank} \bullet b)}{\gamma - 1} - k_{int}A_{int}(T_{wall(int)} - T_{tank})}{\frac{P_{tank}}{\gamma - 1} \bullet b + c_{p,g} \bullet T_{del}}, \quad (23)$$

where $\frac{dP_{tank}}{dt}$ is the pressure ramp used as a model input parameter.

The hydrogen density in the tank is by definition $\rho_{tank} = \frac{m_{tank}}{V}$. The temperature of the hydrogen inside the tank, T_{tank} , can be calculated using Eq. (1) as

$$T_{tank} = \frac{P_{tank}(1 - b\rho_{tank})}{\rho_{tank}R_{H_2}}. \quad (24)$$

The model implies the unsteady heat conduction through the tank wall that can be found elsewhere [34].

$$\rho_{wall}c_{p,wall}\frac{dT_{wall}}{dt} = \frac{d}{dx} \left(\lambda_{wall} \frac{dT_{wall}}{dx} \right). \quad (25)$$

The conservation of energy requires the equality of the convective heat flux between gas and the wall to the conductive heat flux at the wall boundary. Thus, boundary conditions at internal and external surfaces of the tank are defined by Eq. (26) and Eq. (27) respectively

$$q''_{conduction}(internal) = q''_{convection} \Rightarrow -\lambda_{wall} \left. \frac{dT_{wall(n)}}{dx} \right|_{n=int} = k_{int}(T_{tank} - T_{wall(int)}), \quad (26)$$

$$q''_{conduction\ (external)} = q''_{convection} \Rightarrow -\lambda_{wall} \left. \frac{dT_{wall\ (n)}}{dx} \right|_{n=ext} = k_{ext} \left(T_{wall\ (ext)} - T_{amb} \right).$$

(27)

It was concluded in Refs. [7,21] that in the case of fuelling, the external heat transfer coefficient (k_{ext}) does not have a significant effect. The value of k_{ext} is then accepted to be 6 W/m²/K in our study following [21].

The model input parameters are presented in Table 2. The model can predict the dynamics of gas temperature inside the tank, the temperature profile within the load bearing wall and the liner, the gas density or State of Charge (SOC), etc.

Table 2 Input parameters.

alt-text: Table 2
Tank volume (V)
Co-volume constant for hydrogen in Abel-Noble equation (b)
Specific heats ratio for hydrogen (γ)
Ambient temperature (T_{amb})
Delivery temperature of gas during fuelling as a function of time (T_{del})
Pressure ramp in the tank ($\frac{dP_{tank}}{dt}$)
Hydrogen initial temperature in tank (T_{tank}^0)
Tank wall initial temperature (T_{wall}^0)
Internal tank surface (A_{int})
Wall control volume size (Δx)
Time step (Δt), meeting criteria of $\Delta t < < \frac{1}{2} \bullet \frac{\rho_{wall} \bullet c_{p,wall}}{\lambda_{wall}} \bullet (\Delta x)^2$ [35]
Hydrogen gas constant (R_{H_2})
Wall control volume density ($\rho_{wall(n)}$)
Wall control volume specific heat capacity ($c_{p\ wall(n)}$)
Wall control volume conductivity (λ_{wall})
Convective heat transfer coefficient at external surface of tank wall (k_{ext}), 6 W/m²/K [21]
Nozzle diameter (D_{int})
Internal tank length (L)

Gravity acceleration (g)

Thermal expansion coefficient of gas (β), $\frac{1}{T_{tank}}$

Specific heat capacity of the inside gas at constant pressure ($c_{p,g}$), (see Fig. 2)

Dynamic viscosity of gas (μ_g), (see Fig. 2)

Thermal conductivity of gas (λ_g), (see Fig. 2)

The system of equations is solved iteratively. Before start of the fuelling the mass flow rate $\dot{m}_{inlet}^0 = 0$ kg/s. The convective heat transfer between internal surface of the tank wall and hydrogen gas is only due to natural convection at the start. Initial condition (at iteration number $i = 0$) are then.

$$\begin{aligned} 1 \quad & \rho_{tank}^0 = \frac{p_{tank}^0}{p_{tank}^0 \cdot b + R_{H_2} \cdot T_{tank}^0} ; \\ 2 \quad & m_{tank}^0 = V \cdot \rho_{tank}^0 ; \\ 3 \quad & Nu_{int\ natural}^0 = 0.104 \times \left(\frac{g\beta |T_{tank}^0 - T_{wall(int)}^0| c_{p,g} (\rho_{tank}^0)^2 D_{int}^3}{\mu_g \lambda_g} \right)^{0.352} ; \\ 4 \quad & k_{int\ natural}^0 = \frac{\lambda_g \cdot Nu_{int\ natural}^0}{D_{int}} . \end{aligned}$$

After defining initial conditions ($i = 0$), the iteration number is updated (step 1, Fig. 3) and calculation starts with $i = 1$. Fig. 3 demonstrates the iterative procedure to solve the system of equations. Each iteration starts by updating the iteration number (transition to new time by adding time step to previous time). The mass and the temperature in the tank are calculated at step 2 by using the key input parameter for the development of fuelling protocol, i.e. the pressure ramp in the tank, $\frac{dp_{tank}}{dt}$, which is a function of time. Then, the wall and its internal and external surfaces' temperature are calculated in step 3. Step 4 includes calculation of the characteristic velocity in the tank. Then calculation of internal heat transfer coefficient for natural or forced convection is done at step 5. The regime of convection is defined in step 6 with respect to values of Gr_{tank} and Re_{tank} . The stopping criterion is defined based on not violating the maximum temperature, pressure and SOC prescribed by the regulation [1-4].

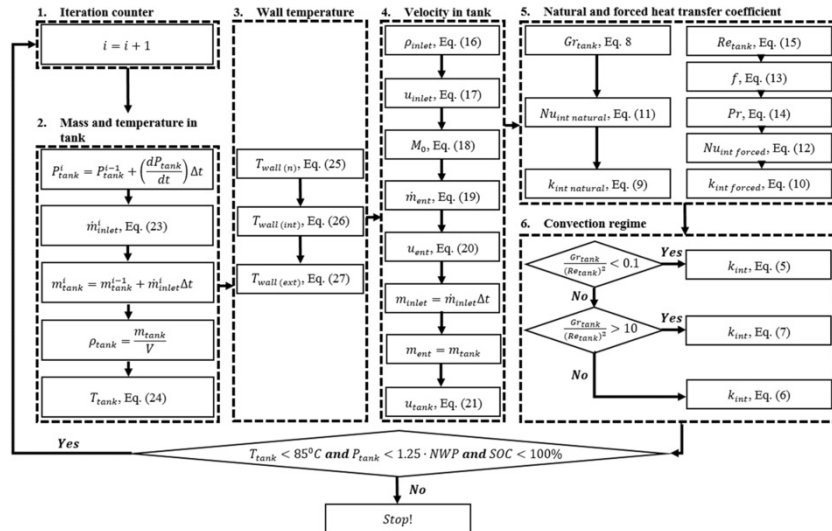


Fig. 3 Iterative procedure to solve the system of equations.

alt-text: Fig. 3

Validation experiments

Three hydrogen tank fuelling experiments [6,7] were selected for the validation of the physical model of fuelling developed in this study. Table 3 presents the characteristics of the experimental tanks. The details of experiments were out of scope of the current study and they are available in Ref. [6] for the 29 L, Type IV tank and 40 L, Type III tank, and in Ref. [7] for the 74 L, Type III tank. According to Ref. [6], for 29 L volume Type IV tank and 40 L volume Type III tank, the measurements of gas temperature inside the tank were done by 8 thermocouples. The three tanks were all in horizontal position. It was concluded in Refs. [6,22] that five out of 8 thermocouples, i.e. in the middle of the tank from top to bottom, were assigned to be used for the averaging the temperature due to having same temperature trend (with the maximum temperature difference of 3 °C). Sixteen thermocouples were used to measure gas temperature inside the 74 L volume Type III tank in experiment [7]. There is no information in Ref. [7] how the temperatures were averaged (however, it is mentioned that the maximum difference of gas temperature measured by different thermocouples was 5 °C). Table 3 shows that for 74 L volume Type III tank [7], the filling time is 640 s, i.e. longer compared to the consumers' expectations of 3 min. However, it is selected as a validation experiment to demonstrate the capability of the physical model to predict experimentally measured temperatures when the pressure ramp (input parameter of the model) is not constant as in fuelling tests of 29 L volume Type IV tank and 40 L volume Type III tank [17], but is changing from higher to lower value during fuelling in this test with 74 L volume Type III tank [7].

Table 3 Characteristics of tanks used in validation experiments [6,7,26].

alt-text: Table 3

Characteristics	Type IV	Type III	Type III
Reference	[6]	[6]	[7]
Volume (L)	29	40	74
External length (mm)	827	920	1030
External diameter (mm)	279	329	427
Internal diameter (mm)	230	290	354
Liner material:	HDPE ^a	AA ^a	AA ^a
$\lambda_{wall\ (liner)}$ (W/m/K)	0.385	167	238
$c_{p\ wall(liner)}$ (J/kg/K)	1580	900	902
$\rho_{wall(liner)}$ (kg/m ³)	945	2700	2700
Composite shell (wall) material:	CFRP	CFRP	CFRP
$\lambda_{wall\ (CFRP)}$ (W/m/K)	0.74	0.74	0.612
$c_{p\ wall\ (CFRP)}$ (J/kg/K)	1120	1120	840
$\rho_{wall\ (CFRP)}$ (kg/m ³)	1494	1494	1570
Injector (inlet) diameter (mm)	3	3	5
Ambient temperature (K)	293	293	303
Initial temperature (K)	293	293	288
Gas delivery temperature (K)	298	298	270

Initial hydrogen pressure (MPa)	2	2	5.5
Target pressure (MPa)	77	77	70
Filling time (s)	250	420	640

^a HDPE: high density polyethylene; AA: aluminium alloy; CFRP: carbon fibre reinforced polymer.

Results and discussion

Figs. 4–6 demonstrate good agreement of simulated by the model hydrogen temperature dynamics inside a tank against the validation fuelling experiments for 29 L Type IV tank [6], 40 L Type III tank [6] and 74 L Type III tank [7] respectively. The figures show as well temperature of inner surface of a liner. The pressure ramp in each experiment is shown in Figs. 4a, 5a and 6a. These pressure ramps were applied in the physical model as inputs. Employing Eq. (23), the simulated mass flow rates in each validation experiment are presented in Figs. 4b, 5b and 6b. It is worth to mention that in all three cases the maximum mass flow rate is less than 60 g/s which is the maximum permissible mass flow rate according to Ref. [3]. To demonstrate the ability of the model to simulate the temperature evolution within the tank wall, the simulated temperature at the inner surface of the tank wall is also presented in Figs. 4c, 5c and 6c along with the gas temperature.

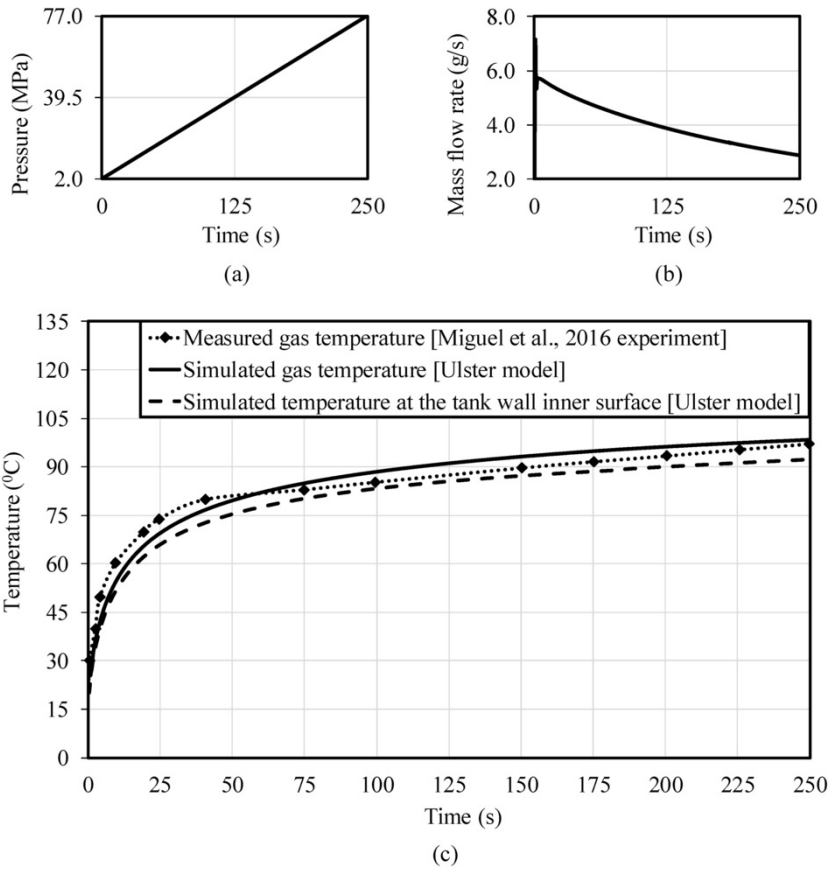


Fig. 4 (a) - Pressure ramp inside the tank used as input data; (b) - Simulated mass flow rate inside the tank; (c) - Experimental and simulated temperature dynamics for the Type IV tank, 29 L [6].

alt-text: Fig. 4

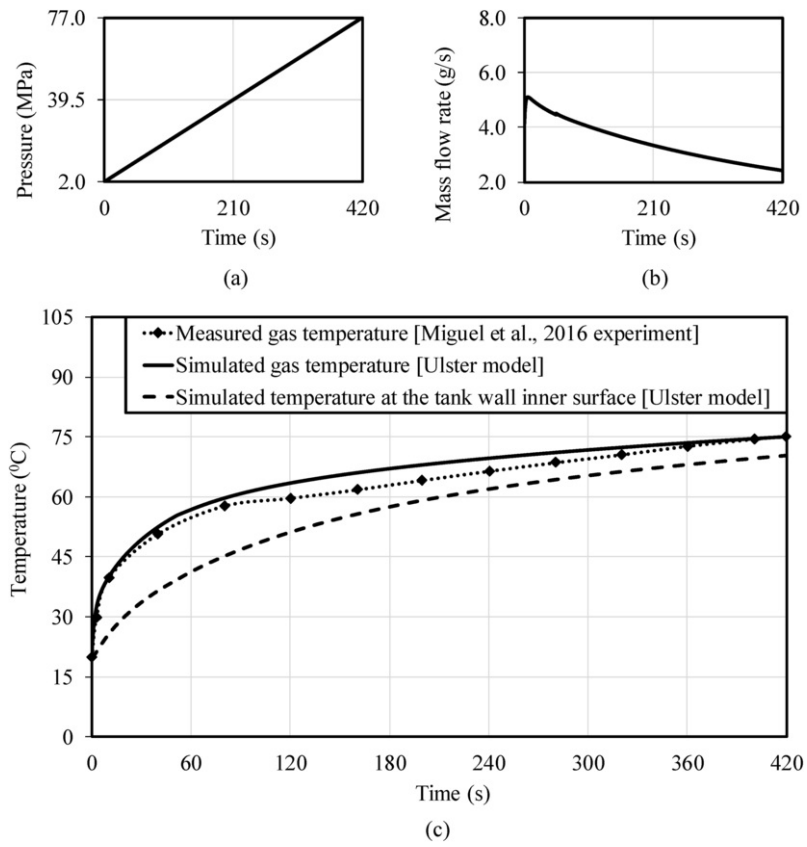


Fig. 5 (a) - Pressure ramp inside the tank used as input data; (b) - Simulated mass flow rate inside the tank; (c) - Experimental and simulated temperature dynamics for the Type III tank, 40 L [6].

alt-text: Fig. 5

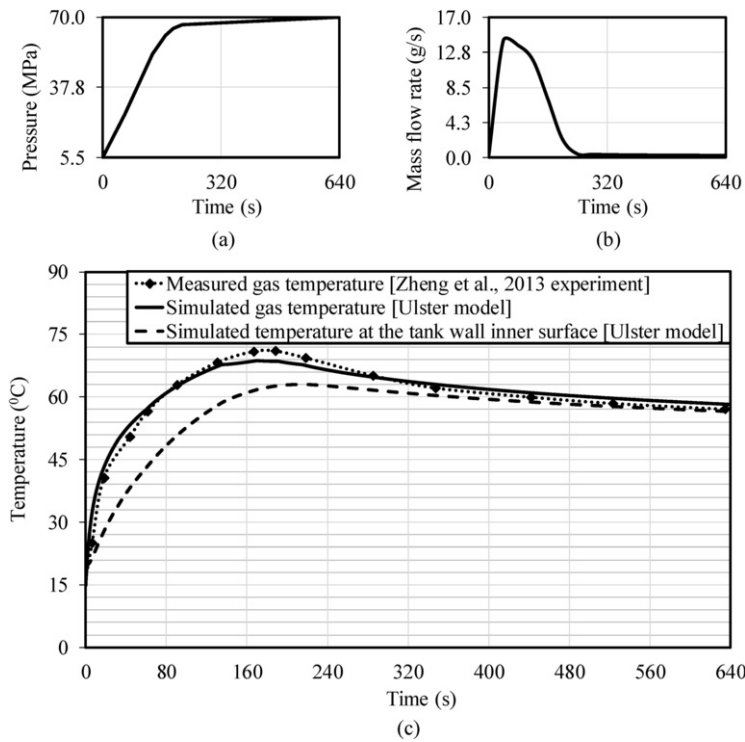


Fig. 6 (a) - Pressure ramp inside the tank used as input data; (b) - Simulated mass flow rate inside the tank; (c) - Experimental and simulated temperature dynamics for the Type III tank, 74 L [7].

alt-text: Fig. 6

In the case of the smallest tank of volume 29 L (Fig. 4), the model slightly underpredicts the experimental gas temperature at the beginning of the process (0–60 s), and the calculations are more accurate to the end of the fuelling. The calculated value of SOC at the end of simulation was 90%, however the simulation was stopped after 250 s as per the experiment duration.

The model slightly overpredicts temperature for fuelling test with 40 L volume Type III tank (Fig. 5). It is worth mentioning that in this validation test the pressure ramp was lower compared to the first validation test. Though the calculated value of SOC was 94%, the simulation was terminated at 420 s (the duration of this experiment).

In both cases (29 L Type IV and 40 L Type III tanks) the maximum deviation of the simulated temperature from the experimental temperature is below 5 °C. The maximum experimental temperature difference in the tank is reported as 3 °C [22]. This confirms that the simulation results are in a good agreement with the experimental data.

In the case of the largest 74 L volume Type III tank fuelling (Fig. 6), the model slightly overpredicts at the beginning, but then slightly underpredicts when the simulation continues to the end of the test. In this validation experiment the pressure ramp was changing during fuelling opposite to the constant pressure ramp (but different) applied in two previous tests. The pressure ramp is significantly higher at the beginning of the fuelling and the pressure ramp slope reduces significantly after around 160–180 s. The result is the temperature peak in the temperature dynamics. The SOC value of 92% is obtained at the end of the simulation when the fuelling time reached 640 s as in the experiment. The maximum deviation of the simulation in Fig. 6 is again 3 °C. According to Ref. [7], the maximum experimental difference in the tank is 5 °C which makes an excellent agreement between the simulated temperature and that obtained in the experiment.

The model reproduces the experimental gas temperature peak (see Fig. 6). The model demonstrates the predictive capability to simulate the dynamic behaviour of the pressurised tank during hydrogen refuelling: predicting dynamic temperature of the gas inside the tank, temperature evolution within the tank wall, mass flow rate and final SOC by using the pressure ramp inside the tank as an input as per available validation experiments. Further research and the model capability expansion will be based on more “realistic” experiments with piping and fuelling conditions closer to the real world compressed hydrogen refuelling condition. The ultimate target is to develop a time efficient and accurate model enabled to predict dynamic behaviour of the tank by employing the gas pressure ramp and gas delivery temperature. This would require the communication between a vehicle and refuelling station to provide

inherently safer for customers fuelling. The equipment to transfer of hydrogen from the storage through piping, valve, breakaway, hose and nozzle have to be included into the model.

Conclusions

The significance of this study is in the development of the model accounting for all main underlying physical phenomena during hydrogen fuelling of composite onboard high-pressure cylinders that can be used for the development of automated hydrogen fuelling protocols for vehicles. The model provides the essential parameters for the regulatory control of the thermal behaviour of the tank during the fuelling, including but not limited to gas temperature, pressure and the state of charge, etc. Further research should develop criteria for gas temperature uniformity inside the tank to apply the model for heavy-duty vehicles with larger onboard storage tank volume.

The rigour of the study is in the model validation against experimental data on fuelling of hydrogen storage tanks of Type III and Type IV of volumes in the range 29–74 L up to pressure 77 MPa with constant and changing during fuelling pressure ramp. The model reproduces experimental temperature dynamics within acceptable maximum deviation value of 5 °C, which is characteristic for hydrogen temperature non-uniformity measured in fuelling tests.

The originality of this study is based on integrating physics and thermodynamic methods and correlations in one engineering tool to achieve the synergy through their complementarities. The cornerstone of the model is the use of the entrainment theory in combination with conservation of kinetic energy for calculation of gas velocity inside the tank to calculate Reynolds number used in the estimation of Nusselt number and thus the heat transfer coefficient for the forced convective heat transfer between the tank wall and the gas.

The model can be used as a part of expanded model for a system refuelling hydrogen storage-piping-dispenser-onboard storage for the further investigations on thermal behaviour of the system during the fuelling and the development of the fuelling protocol, including effect of pre-cooling.

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Highlights

- Physical model of hydrogen tank thermal behaviour during fuelling is developed.

- The entrainment theory is applied to calculate characteristic velocity in the tank.
 - The model is validated against experiments on fuelling of Type III and IV tanks.
 - The deviation of model prediction of temperature is within experimental scatter 5 °C.
-

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